National Aeronautics and
Space Administration

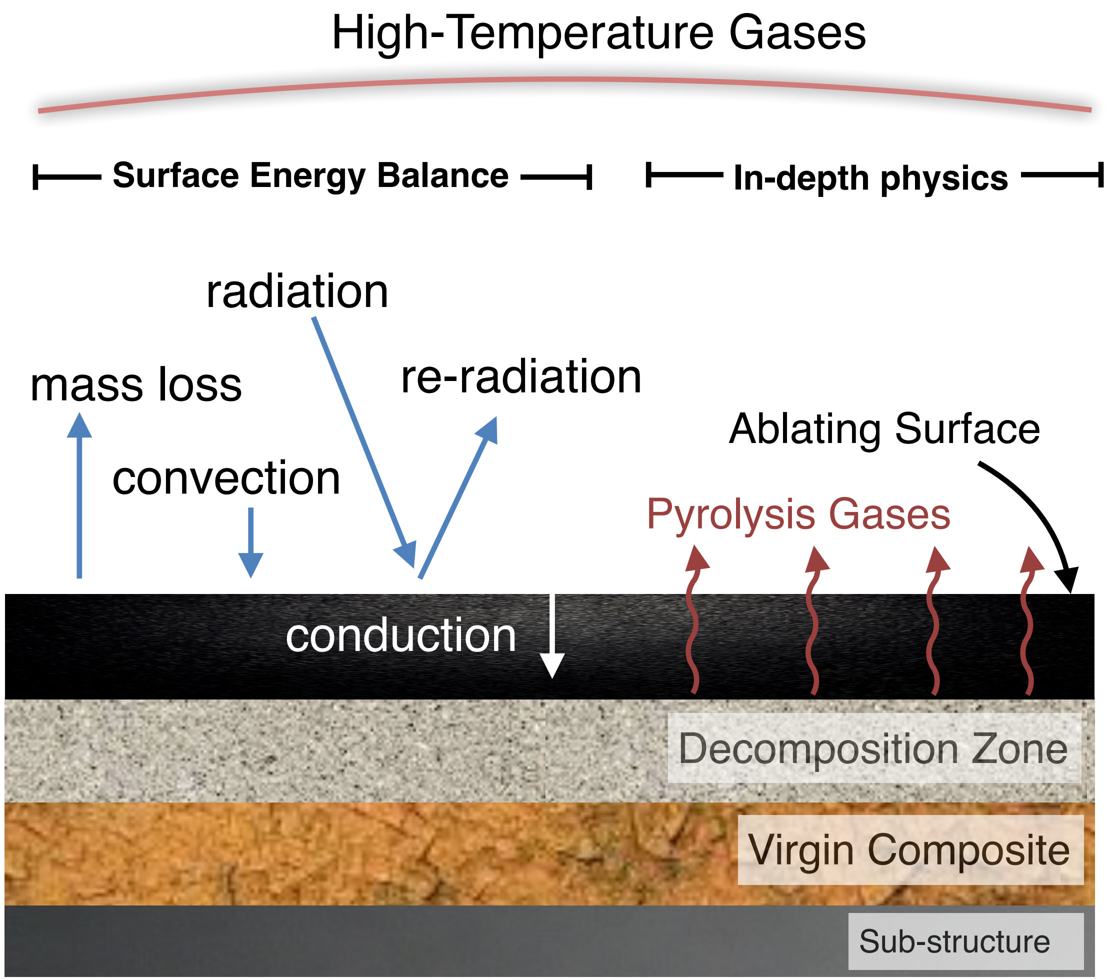
Development of an, unstructured, three-dimensional material response model

AIAA SciTech Conference

Grapevine, TX 2017

Joseph Schulz, Eric Stern, Grant Palmer, Suman Muppidi, Olivia Schroeder, and Alexandre Martin

Background



NASA Material Response Tools

<u>*Engineering Tools*</u>
- STAB / CHAR *(NASA JSC)*
- FIAT / TITAN *(NASA ARC)*
- **Icarus *(NASA ARC)***

⇧ *Inform engineering models*

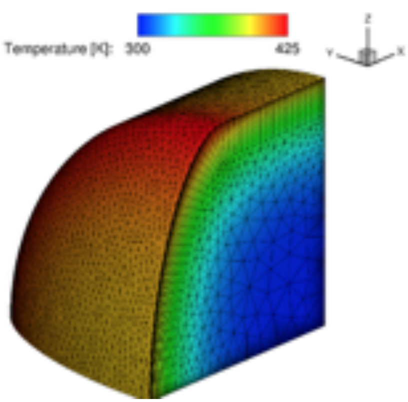
<u>*Research Tools*</u>
- PATO *(NASA ARC)*

<u>*Material Properties*</u>
- PuMA *(NASA ARC)*

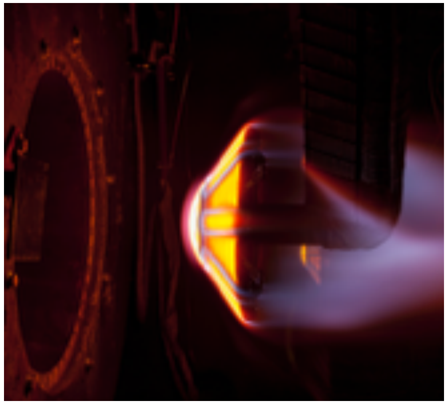
*Not an exhaustive list

Motivation

- **Why Icarus?**
  - Three-dimensional physics modeling and complex geometries
  - Coupling to CFD simulation
  - Software architecture
    - ➢ Easy to add new physics, numerics, and material property models
    - ➢ Linking to optimization and inverse parameter estimation methods
  - Independent of other NASA material response models
    - ➢ Provides verification of predictions
- **Target Applications**



3D ArcJet IsoQ



ADEPT ArcJet Test

Orion Compression Pad

Icarus

Spring 2017 | Winter 2017

ICARUS
Development Roadmap

Version 1.0

Physics Models
Thermal Conduction
+ Decomposition
+ Pyrolysis Gas Continuity

Numerical Methods
Time integration
- First-order Backward Euler
- Second-order Runge-Kutta
Spatial integration
- Green-Gauss reconstruction
Mesh Motion
- Radial-basis functions

Verification and Validation
Analytical Heat Conduction
Ablation Workshop Test Cases
PICA ArcJet validation

Version 2.0

Physics Models
Thermal Conduction
+ Pyrolysis Gas Momentum
+ Element Conservation

Numerical Methods
Implicit Time Integration
- Point relaxation
- Numerical Jacobians
Gradient reconstruction
- Weighted least-squares

Verification and Validation
Orion ArcJet validation
HEEET ArcJet validation
MSL Flight data

Version 3.0

Physics Models
Dust erosion / spallation
Linear elasticity model

Numerical Methods
AMR

Interface
GUI
Design Toolbox
- Shape optimization
- Inverse parameter estimation
- Uncertainty quantification

Icarus - Version 1.0 Status

Indicates an external binary

***Indicates a work in progress**

Input / Output Data Formats
HDF5 / XDMF, CGNS, Tecplot

Data I/O and Initialization

Main Loop

finish

Data I/O and Post-processing

Thermodynamics / Transport

Materials
Icarus Tables / Polynomials

Gas Mixtures
Icarus / NASA CEA
Mutation++
Cantera

Numerics

Explicit Time Integration
First-order Euler
2^{nd}-order Runge-Kutta

Gradient Reconstruction
Green-Gauss contour integration

Physics Models
Heat Conduction
+ Decomposition
+ Pyrolysis gas production
+ Surface recession / ablation

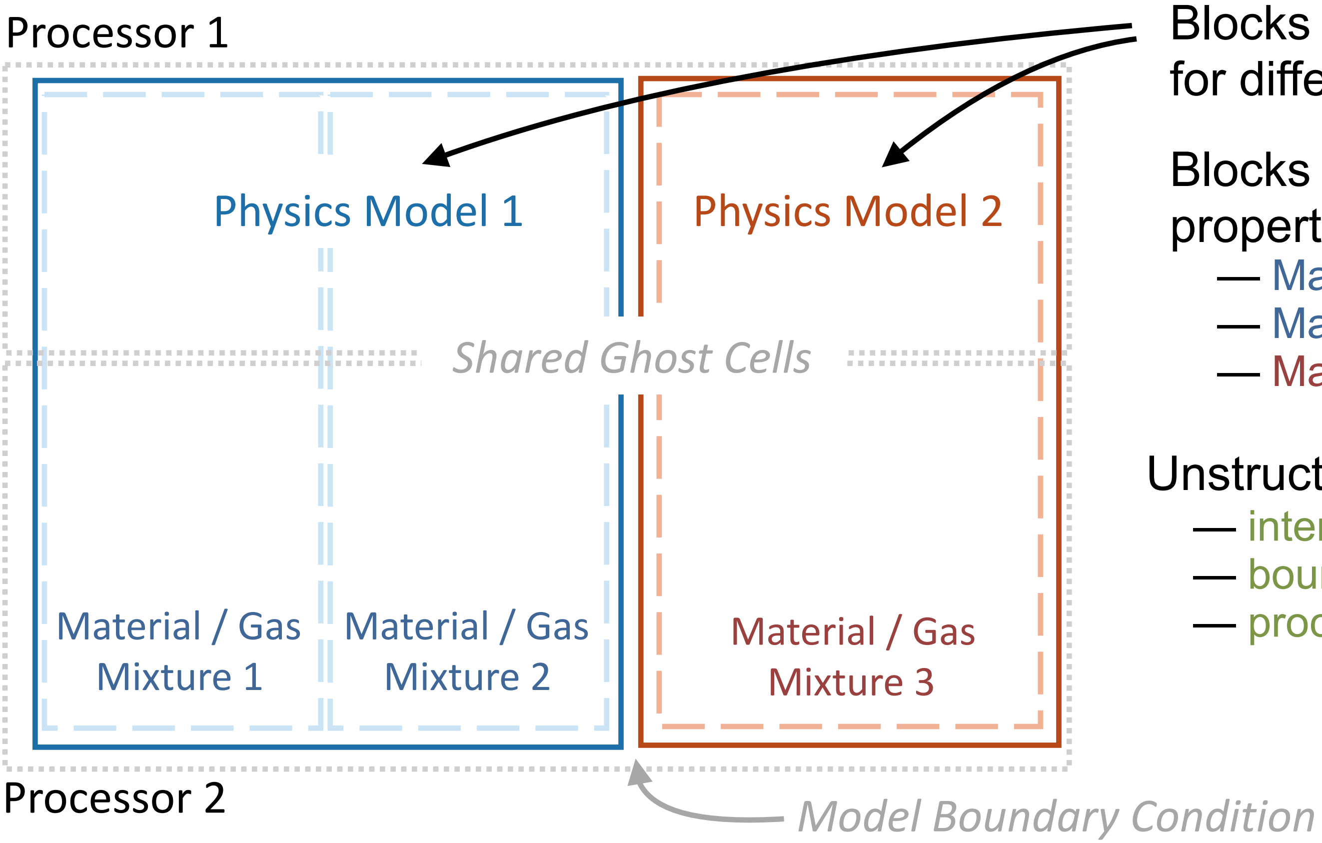
Thermal Boundary Conditions
Isothermal
Heat Flux
- Adiabatic
- Spatial / Temporal Function
Surface Energy Balance

Utilities
Database Creation
Grid Deformation
Icarus GUI

Test Automation
Unit Testing
Integration Testing
Regression Testing

Icarus - Data Structure

- **Modular data structure partitions physics, numerics, and material or gas models**
  - **Organization is user friendly and extensible**



Blocks 1 and 2 are defined for different physics models

Blocks can contain multiple property zones:
- Material / Gas 1
- Material / Gas 2
- Material / Gas 3

Unstructured index ordering
- interior faces / cells
- boundary faces / cells
- processor shared faces / cells

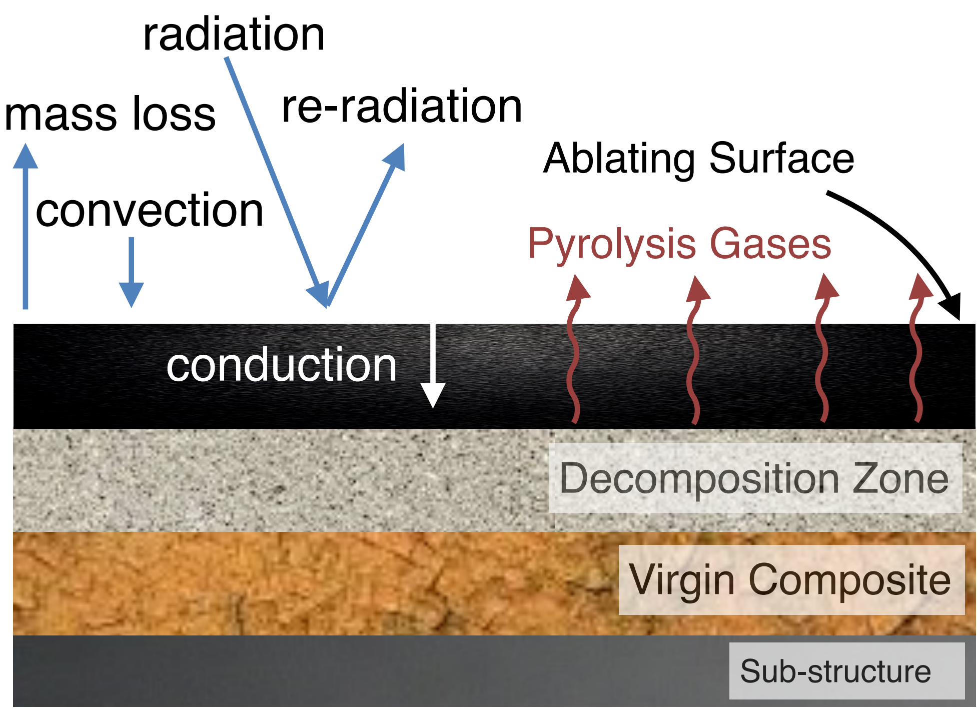
Icarus - Production Code

- **Production codes require :**
  1. Sufficient documentation
     - Web-based documentation
     - Uses Sphinx, a Python tool that parses in-source code documentation to create HTML and LaTeX formatted documentation
  2. Verification
     - Automated unit and integration testing (~60% coverage currently)
     - Regression testing
  3. Validation
     - Comparison to Arc Jet data (current focus of PICA validation)
     - Shifting focus this year to AVCOAT modeling
     - MSL flight data
- **Participation in code-to-code comparisons to understand variability in modeling assumptions and prediction uncertainty**
  - Ablation Workshop
  - Relationships with research institutes and university laboratories

Outline

- **Icarus Formulation**
  - Governing equations
  - Numerical formulation

- Verification Tests
  - Analytical heat conduction
  - Multi-dimensional test cases
- Current On-Going Work
  - Mesh motion
  - Surface ablation



$$\frac{\partial \rho_{s,n}}{\partial t} = -k_n \rho_{v,n} \left(\frac{\rho_k - \rho_{c,n}}{\rho_{v,n}} \right)^{\psi_n} e^{(-T_{a,n}/T)}$$

$$\frac{\partial (\phi \rho_g)}{\partial t} + \frac{\partial}{\partial x_i} \left(\phi \rho_g u_{g,i} \right) = \dot{\omega}$$

$$\frac{\partial (\rho e)}{\partial t} + \frac{\partial}{\partial x_i} \left(\phi \rho_g h_g u_{g,i} \right) - \frac{\partial}{\partial x_i} \left(\kappa_{ij} \frac{\partial T}{\partial x_j} \right) = 0$$

Formulation : Pyrolysis

- **Pyrolysis Modeling**
  1. Solve the elemental conservation equations
     - Requires a detailed kinetic mechanism and knowledge of material composition
  2. Use empirical relationships
     - Measure quantities only at the virgin and fully-charred states
     - Use simplified kinetics
- **Three-component model**

virgin ⇨ ***resin*** + ***binder***

⇩

gas

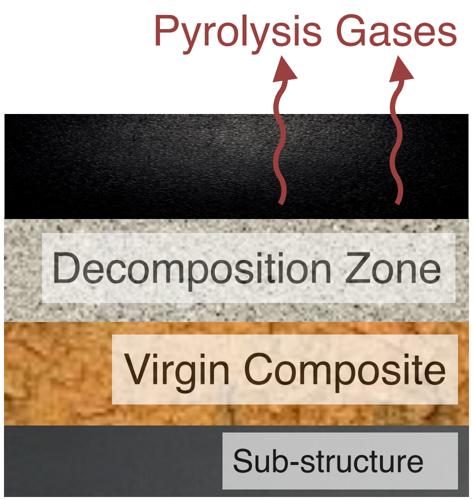
$$\rho_s = \Gamma\left(\rho_A + \rho_B\right) + \left(1 - \Gamma\right)\rho_C$$

Γ : pseudo-volume fraction of pyrolyzing resin

$\rho = \phi\rho_g + \rho_s$; ϕ is the material porosity

$$\frac{\partial \rho_{s,n}}{\partial t} = -k_n \rho_{v,n} \left(\frac{\rho_{s,n} - \rho_{c,n}}{\rho_{v,n}}\right)^{\psi_n} \mathrm{e}^{(-T_{a,n}/T)},$$

$$\omega = \sum_{n=1}^{N} \Gamma_n \frac{\partial \rho_{s,n}}{\partial t}$$: total production of pyrolysis gas



Formulation : Material Properties

- **Properties are measured for at the virgin and fully-charred states**
  - Requires linearly interpolating between two states

$$\beta = \frac{\rho_v - \rho_s}{\rho_v - \rho_c} \longrightarrow Y_v = \frac{\rho_v}{\rho_v - \rho_c}\left(1 - \frac{\rho_c}{\rho_s}\right)$$

  - Internal energy of the material is evaluated either as a tabular or polynomial curve-fit that is a function of temperature and pressure

$$e_s(p,T) = h_s(p,T) = Y_v e_v(p,T) + (1 - Y_v) e_c(p,T)$$

- **Total mixture quantities are determined by weighted average using the gas mass fraction**

$$e(p,T) = Y_g e_g(T) + (1 - Y_g) e_s(p,T) \qquad Y_g = \frac{\phi \rho_g}{\rho}$$

: mass fraction of the gas mixture

- **Thermal equilibrium and gas mixture in chemical equilibrium**

Formulation : Material Properties

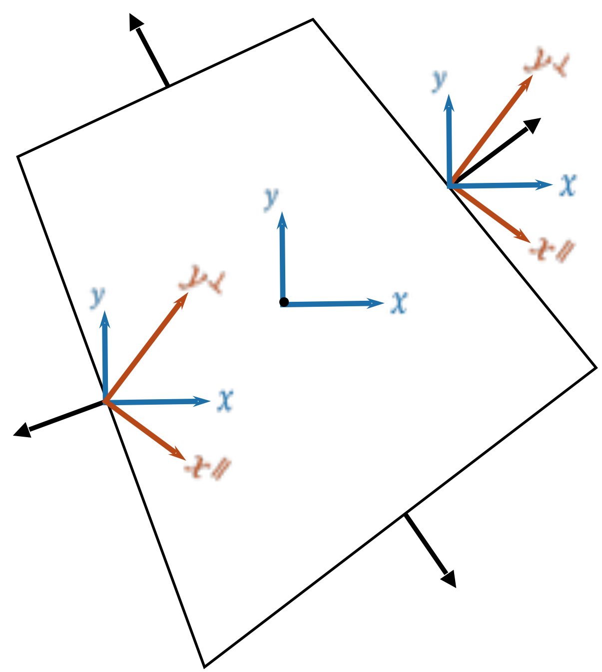
- **Material properties can be orthrotropic**
  - Principle axis of the material may not align with the Cartesian frame of reference of the simulation
    - ➢ Woven TPS materials : alignment varies continuously
- **Properties defined parallel and orthogonal to the principle axis**

Thermal conductivity tensor in material frame of reference

$$\kappa_{ij} = \begin{bmatrix} \hat{\kappa}_{||} & 0 & 0 \\ 0 & \hat{\kappa}_{\perp} & 0 \\ 0 & 0 & \hat{\kappa}_{\perp} \end{bmatrix}$$

Project tensor onto the surface defined by the normal vector at each grid point

$$\boldsymbol{\kappa} = \mathbf{R}^{\mathrm{T}} \hat{\boldsymbol{\kappa}} \mathbf{R}$$



Formulation : Conservation Equations

Decomposition of solid material

$$\frac{\partial \rho_{s,n}}{\partial t} = -k_n \rho_{v,n} \left(\frac{\rho_{s,n} - \rho_{c,n}}{\rho_{v,n}} \right)^{\psi_n} \mathrm{e}^{(-T_{a,n}/T)}, \qquad n = 1, \ldots, N$$

Pyrolysis gas continuity

$$\frac{\partial \left(\phi \rho_g \right)}{\partial t} + \frac{\partial}{\partial x_i} \left(\phi \rho_g u_{g,i} \right) = \dot{\omega}$$

Momentum conservation : Darcy's Law

$$\boxed{u_{g,i} = -\frac{1}{\mu} K_{ij} \frac{\partial p}{\partial x_j}}$$

Total Energy conservation

$$\frac{\partial \left(\rho e \right)}{\partial t} + \frac{\partial}{\partial x_i} \left(\phi \rho_g h_g u_{g,i} \right) - \frac{\partial}{\partial x_i} \left(\kappa_{ij} \frac{\partial T}{\partial x_j} \right) = 0$$

convection of heat by pyrolysis gases

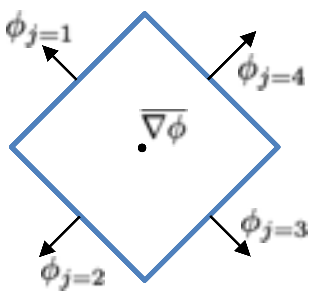
thermal conduction by material

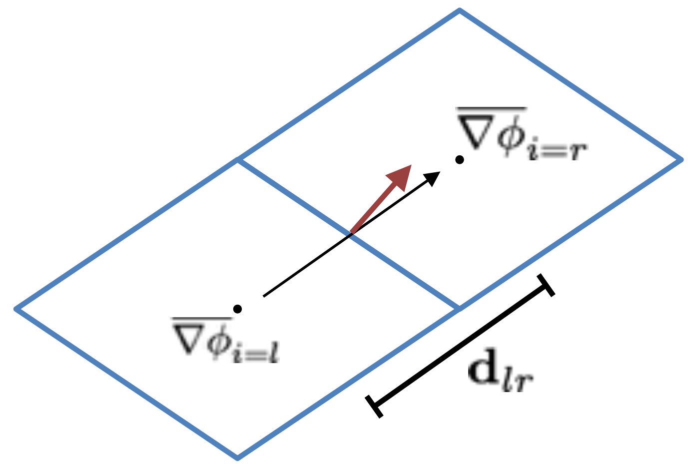
Formulation : Numerics

- **Time integration**
  - Explicit first-order Euler or second-order Runge-Kutta
- **Gradient Reconstruction**
  - Gauss-Green contour integration

$$\int_{\mathcal{V}} \nabla\phi \mathrm{d}\mathcal{V} = \int_{\mathcal{S}} \phi \mathbf{n} \cdot \mathrm{d}\boldsymbol{\mathcal{S}}$$

$$\overline{\nabla\phi}_{\mathrm{i}} = -\frac{1}{\mathcal{V}_{\mathrm{i}}} \sum_{\mathrm{j}\in J_{\mathrm{i}}} \widehat{\phi}_{\mathrm{j}} \mathcal{S}_{\mathrm{i,j}}$$





Average the cell-centered gradients neighboring each face

$$\nabla\phi_{\mathrm{j}} = \frac{1}{2}\left(\overline{\nabla\phi}_{\mathrm{i}=l} + \overline{\nabla\phi}_{\mathrm{i}=r}\right) - \widehat{\mathbf{d}}_{lr}\left(\frac{1}{2}\left(\overline{\nabla\phi}_{\mathrm{i}=l} + \overline{\nabla\phi}_{\mathrm{i}=r}\right)\cdot\widehat{\mathbf{d}}_{lr}\right) + \left(\phi_{\mathrm{i}=l} - \phi_{\mathrm{i}=r}\right)\frac{\widehat{\mathbf{d}}_{lr}}{|\mathbf{d}_{lr}|}$$

Outline

- **Verification Tests**
  - Analytical heat conduction comparisons
  - Determine scheme accuracy
- **Multi-dimensional test cases**
  - Qualitative verification
  - Code-to-code comparisons

- **Current On-Going work**
  - Mesh motion
  - Surface ablation
- **Conclusions**

One-dimensional Analytical Solutions

- **Analytical solutions exist for the one-dimensional heat conduction equation**
  - Ignored pyrolysis or surface recession (constant density and volume)
  - Scalar material properties (tensors are isotropic)
- **Conservation equations reduce to a single PDE**
  - Assuming linear temperature-dependent properties:

$$\kappa(T) = \kappa_1 + \frac{\kappa_2 - \kappa_1}{T_2 - T_1}(T - T_1) \qquad c_v(T) = c_{v,1} + \frac{c_{v,2} - c_{v,1}}{T_2 - T_1}(T - T_1)$$

  - Using the variable transformation :

$$\theta = (T - T_1) + \frac{\kappa_2 - \kappa_1}{T_2 - T_1}\frac{1}{2\kappa_1}(T - T_1)^2$$

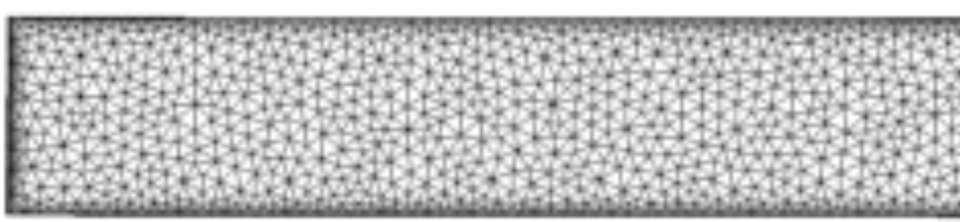
  - Results in:

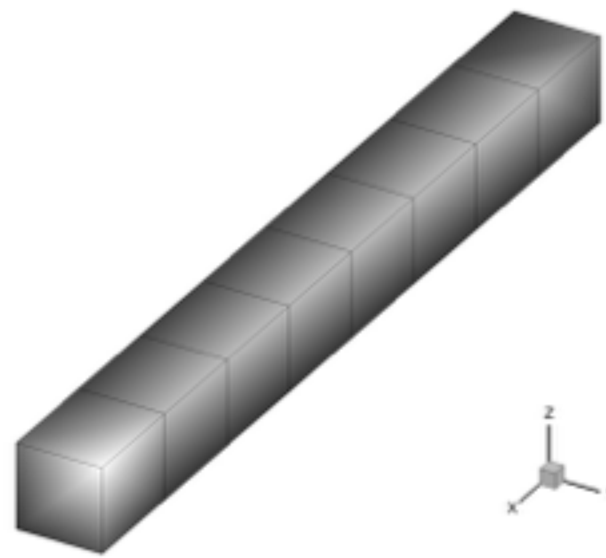
$$\rho c_v \frac{\partial T}{\partial t} - \kappa \frac{\partial^2 T}{\partial x^2} = 0 \longrightarrow \frac{\partial \theta}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

Verification : 1-D Simulation Domain

- **One-dimensional computational domain of 1 m in length**
  - Resolved in the orthogonal directions by 1 grid element
  - Discretization by both triangular prisms and hexahedral elements
- **Estimate the order of accuracy the numerical scheme**
  - Scheme is expected to be second-order accurate
  - Compute the the root-mean-square error (RMS) for an increasing number of grid elements

$$\mathrm{RMS} = \sqrt{\frac{\sum_i^{N_c} \left(T_{\text{analytical}} - T_{\text{numerical}}\right)_i^2}{N_c}}$$

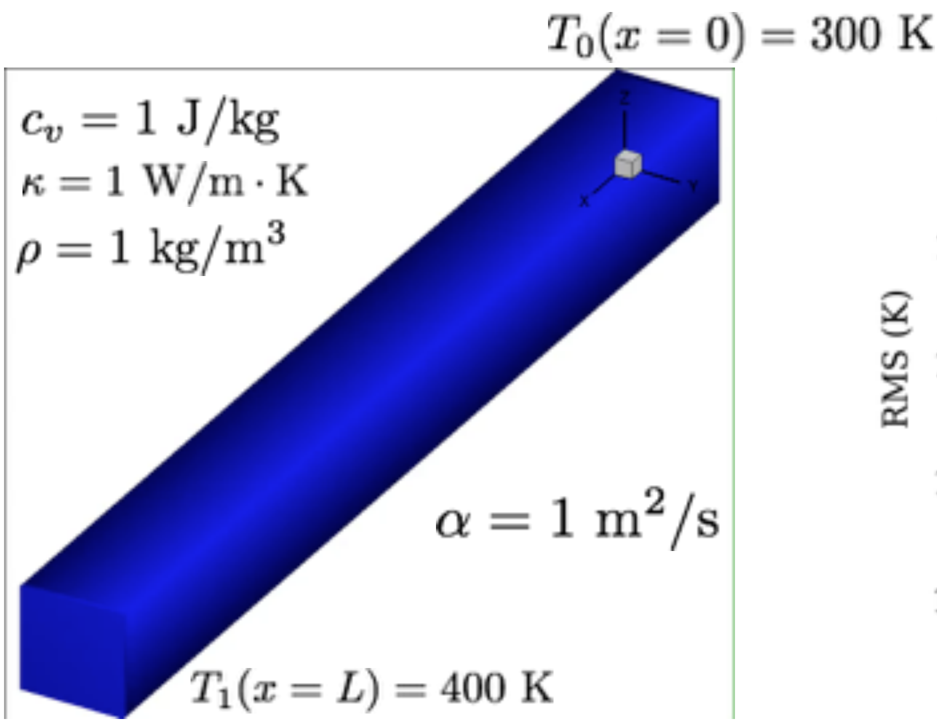


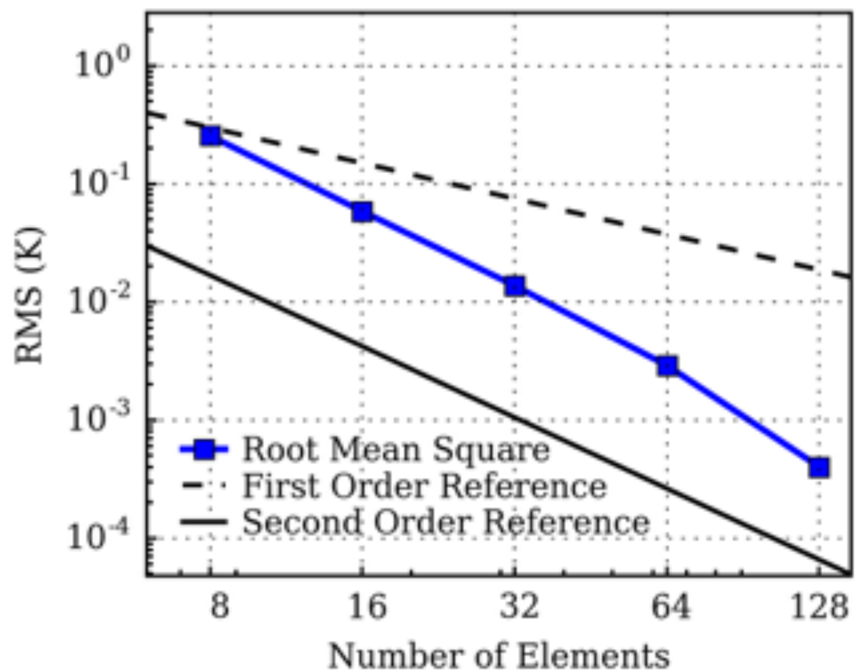


Verification : Analytical Solution #1

- **Isothermal Boundary with constant material properties**
  - Hexahedral elements : 8, 16, 32, 64, and 128

$$\frac{T_1 - T(x,t)}{T_1 - T_0} = 2\sum_{i=0}^{\infty} \frac{(-1)^i}{\left(i+\frac{1}{2}\right)\pi} \exp\left[-\left(i+\frac{1}{2}\right)^2 \pi^2 \frac{\alpha t}{L}\right] \cos\left[\left(i+\frac{1}{2}\right)\frac{\pi x}{L}\right]$$

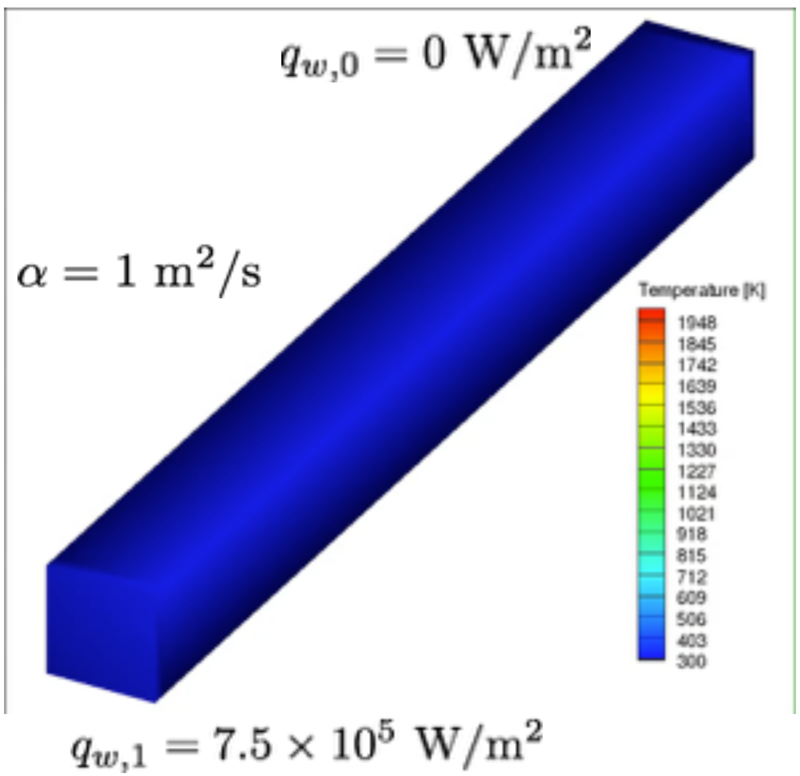


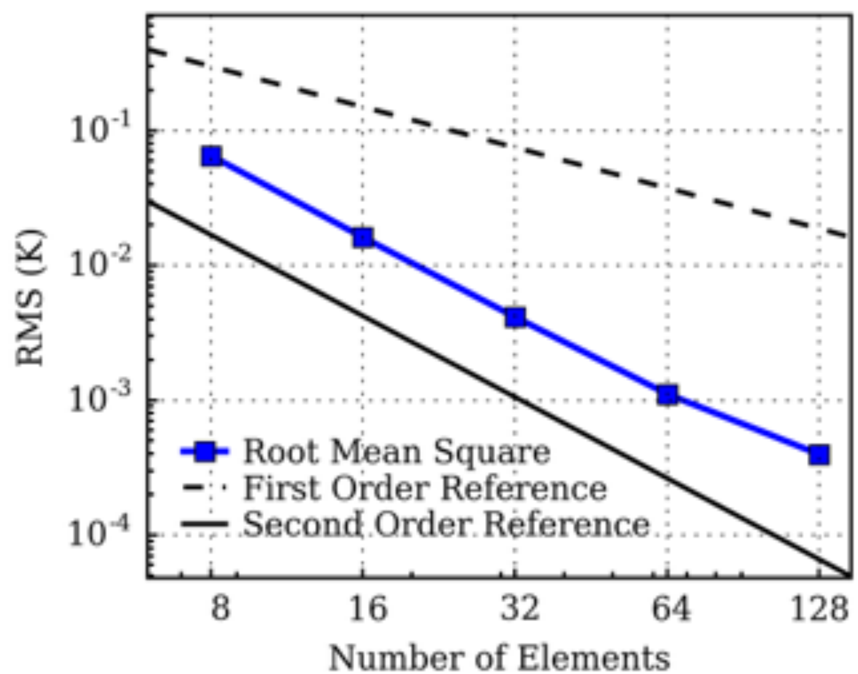


Verification : Analytical Solution #2

- **Constant heat flux boundary and constant material properties**
  - Hexahedral elements : 8, 16, 32, 64, 128

$$\frac{T(x,t)-T_0}{q_{w,1}L/\kappa}=\frac{\alpha t}{L^2}+\frac{1}{3}-\frac{x}{L}+\frac{1}{2}\left(\frac{x}{L}\right)^2-2\sum_{i=0}^{\infty}\frac{1}{n^2}\exp\left[-n^2\pi^2\frac{\alpha t}{L^2}\right]\cos\left[\frac{n\pi x}{L}\right]$$

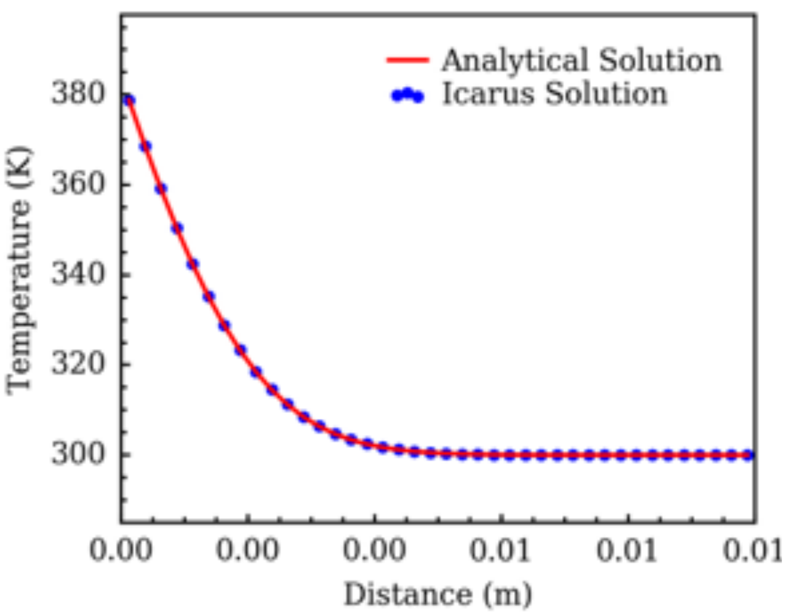


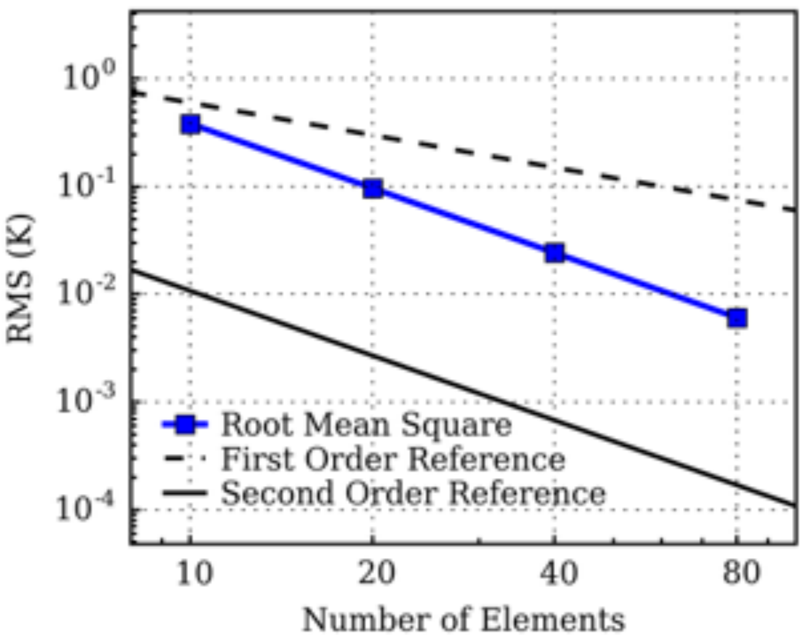


Verification : Analytical Solution #3

- **Constant heat flux with temperature dependent (linear) material properties**
  - Triangular prisms : 10, 20, 40, 80

$$\frac{T(x,t)-T_1}{T_2-T_1} = \left(\frac{\kappa_1}{\kappa_2-\kappa_1}\right)\left[\sqrt{1+\frac{2\theta}{T_2-T_1}\left(\frac{\kappa_2-\kappa_1}{\kappa_1}\right)}-1\right]$$

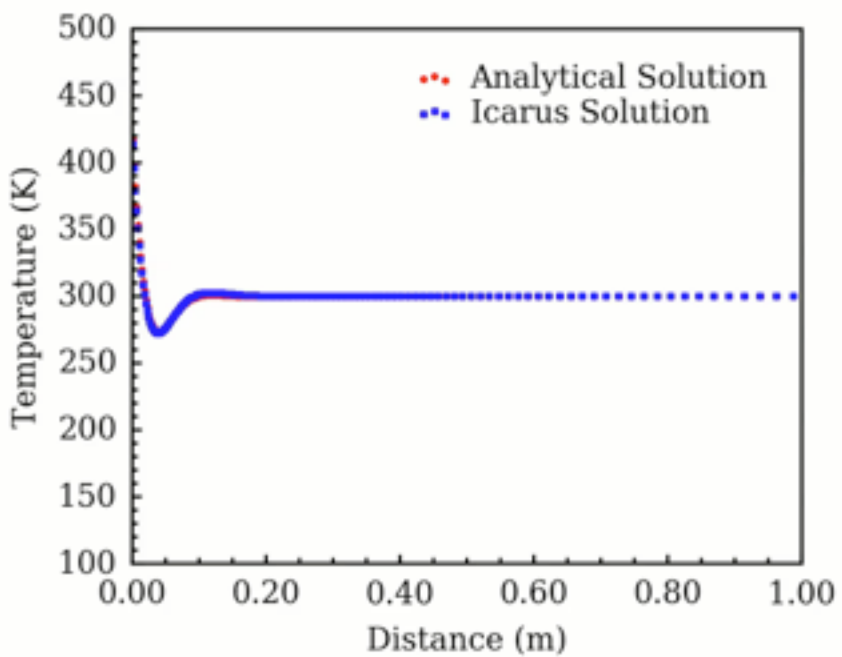


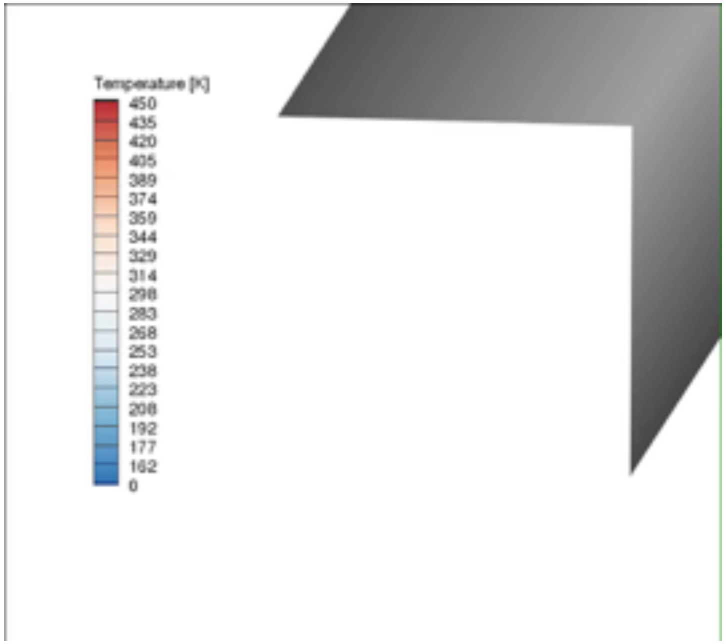


Verification : Analytical Solution #4

- **Sinusoidal varying heat flux boundary with constant material properties**
  - Solution ill-posed since analytical solution exists for semi-infinite domain

$$T(x,t) - T_0 = \frac{q_{w,0}(t)}{\kappa}\sqrt{\frac{\alpha}{\kappa}}\exp\left[-\frac{\omega}{2\alpha x}\right]\cos\left(\omega t - \sqrt{\frac{\omega}{2\alpha}}x - \frac{\pi}{4}\right)$$





Ablation Workshop Test Cases

- **One-dimensional domain : L = 5 cm**
  - Hexahedral elements : 128
- **Boundary conditions**
  - Single isothermal wall

$$T_{x=0} = \begin{cases} 298\,\mathrm{K}: & t \leq 0.1 \text{ sec} \\ 1644\,\mathrm{K}: & t > 0.1 \text{ sec} \end{cases}$$

  - All other boundaries are adiabatic
  - Initial pressure : p = 101325 Pa
- **Material : PICA**
  - Properties are othrotropic
  - Three-component decomposition model

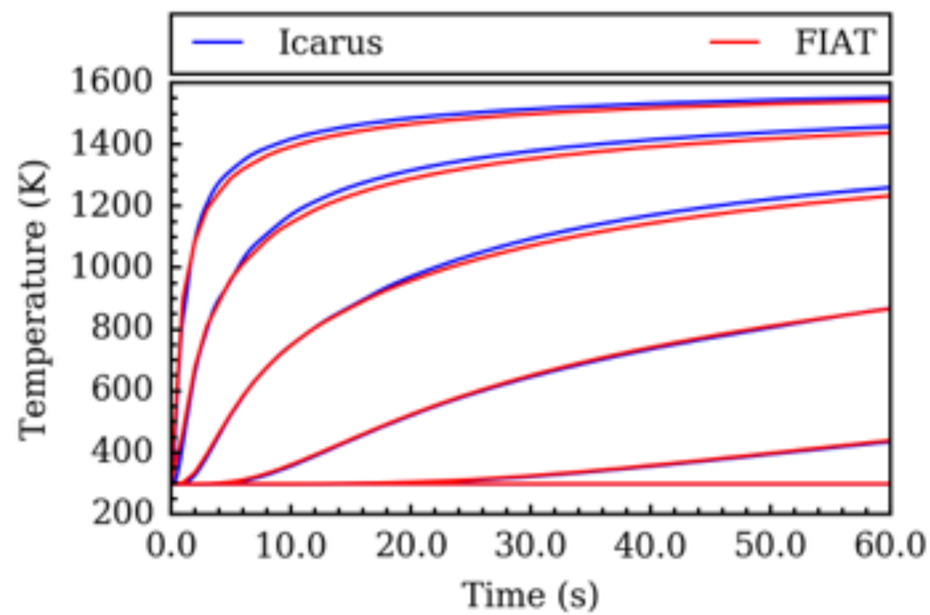


Figure (above) : Code-to-code comparison of Icarus and FIAT for the first ablation workshop test case. Differences are less than 3 percent.

Arc Jet Verification & Validation

- **Three-dimensional iso-q geometry typical of arc jet test articles**

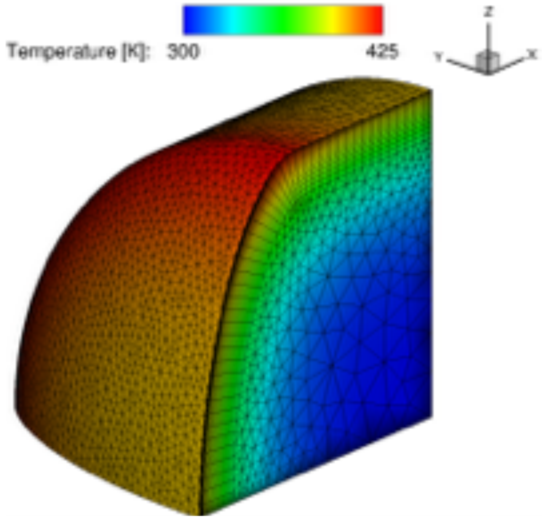
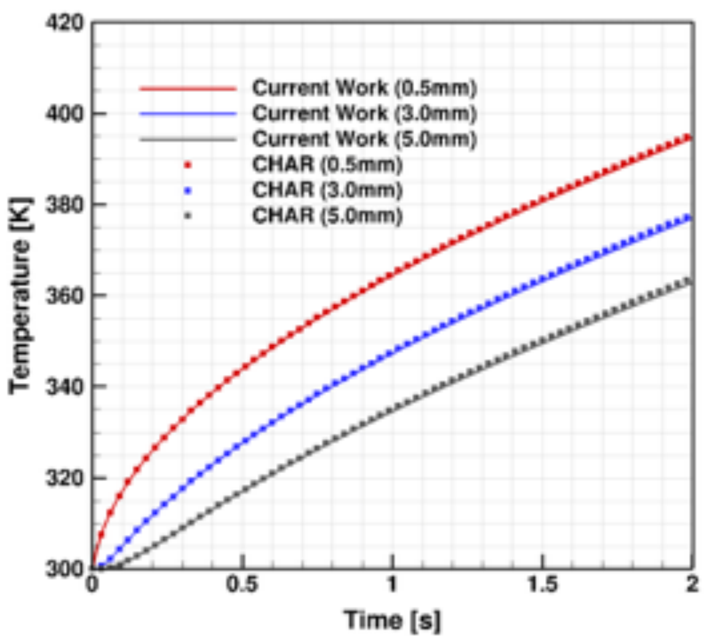


Figure (right) : Temperature contours for Iso-Q geometry heated along the outside radius by a constant heat flux of $q_w = 7.5 \times 10^5 \ \mathrm{W/m^2}$ for TACOT material

Figure (above) : Code-to-code comparison of temperature along the x-axis between Icarus and CHAR



Outline

- Verification Tests
  - Analytical heat conduction comparisons
  - Determine scheme accuracy
- Multi-dimensional test cases
  - Qualitative verification
  - Code-to-code comparisons
- **Work in progress**
  - **Mesh motion / Surface ablation**
  - **Validation**
  - **Release of Icarus v1.0**

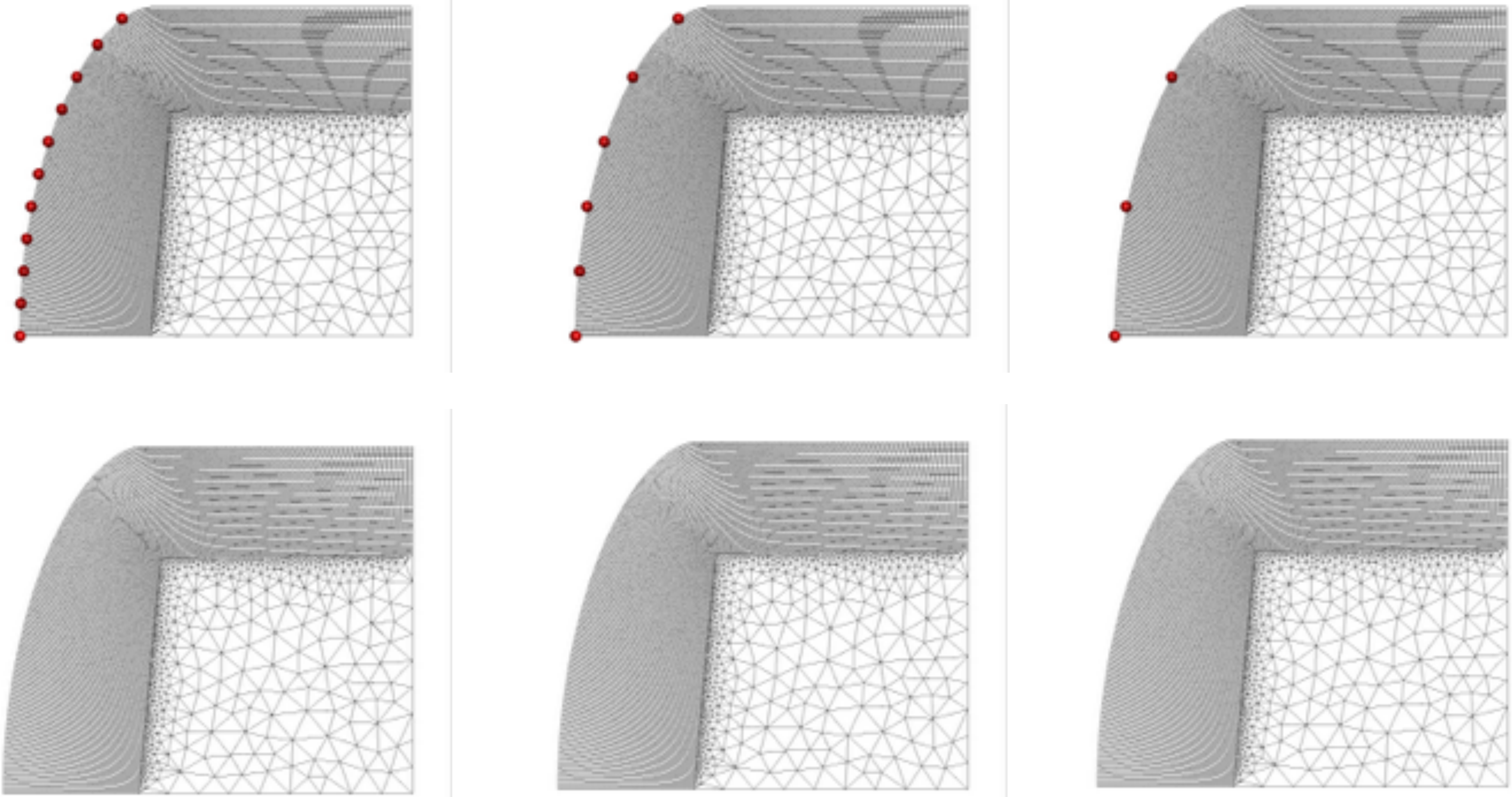
Mesh Motion

- **Ablation results in surface recession**
  - Need a robust and efficient method to track the deformation of the computational grid during the simulation
- **Radial Basis Functions**
  - A real-valued function whose value depends only on absolute distance
  - Often use to approximate functions

$$y(\mathbf{x}) = \sum_{i=1}^{N} w_i \phi\left(|\mathbf{x} - \mathbf{x}_i|\right)$$

  - Here N radial basis functions each weighted differently are used to approximate the function
- **Applications to mesh motion**
  - Define a radial basis function for each grid point with respect to certain control points
  - Compute the weights (requires solving a linear system)

Mesh Motion



Future Work and Conclusions

- Focus on the verification of one-dimensional heat conduction and pyrolysis
  - Numerical scheme
  - Thermodynamic / Transport Properties
  - Grid deformation
- Future Work
  - Validation to arc-jet data and continuation of code-to-code comparisons
  - Addition of surface recession / ablation modeling using radial basis function methodology
  - Integration of inverse estimation and Monte-Carlo analysis tools